Design of a low energy multi-chopper spectrometer on a spallation source
LET

Draft 15 feb 01

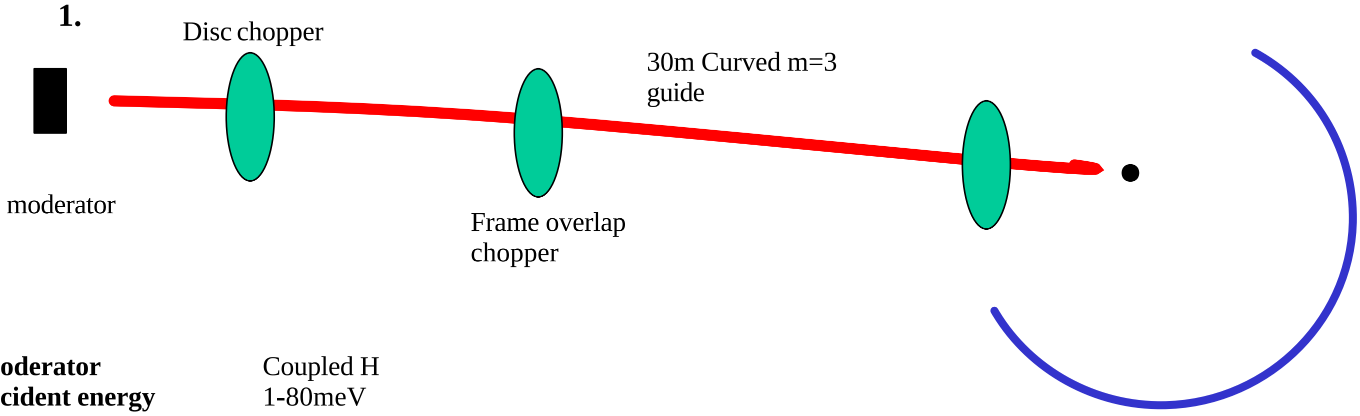
1 Introduction

The aim of this work is to design a multi chopper spectrometer (MCS) optimised for cold neutrons (Ei in range 1-30meV). In this document the instrument will be called LET (Low energy transfer). At present MCS's only exist on reactor sources such as NEAT (HMI) and IN5 (ILL). However, unlike many neutron instruments, the flux on a direct geometry spectrometer is directly related to the peak flux magnitude of the moderator and not the time averaged flux. This vastly favours spallation sources over reactor sources for such an instrument. Results later show that a low energy MCS built at ISIS would easily be the worlds most powerful MCS.

Muti chopper spectrometers also have the advantage of giving the user complete flexibility over resolution and lineshape. The resolution of a direct geomerty spectrometer is essentially defined by two components; the moderator time width and the chopper opening time. On instruments like HET and MAPS one has no control over the moderator component of the resolution (other than deciding on the type of moderator to initially put the instrument on). The resolution can only be controlled by changing the chopper opening time. This not only limits the lowest resolution you can achieve but it also means that the two resolution components are not 'matched' and hence you do not obtain the best possible flux for a particular resolution. A MCS allows you to adjust both of these resolution components and so you can always get close to the optimum flux. The lowest resolution is limited only by the physical limits of the chopper speed.

2 Schematic of a MCS

1.



Moderator	Coupled H
Incident energy	1-80meV
Best resolution	1% at 1meV-5%at 80meV
Primary length	30m
Sample-detector	2.5m
Flight path	m=3 supermirror curved guide
Choppers	2 pairs of counter-rotating disc choppers (5-330Hz)+frame overlap chopper
Detectors	Position sensitive. Angular range -30 to 150 degrees

2 Instrument Energy Resolution

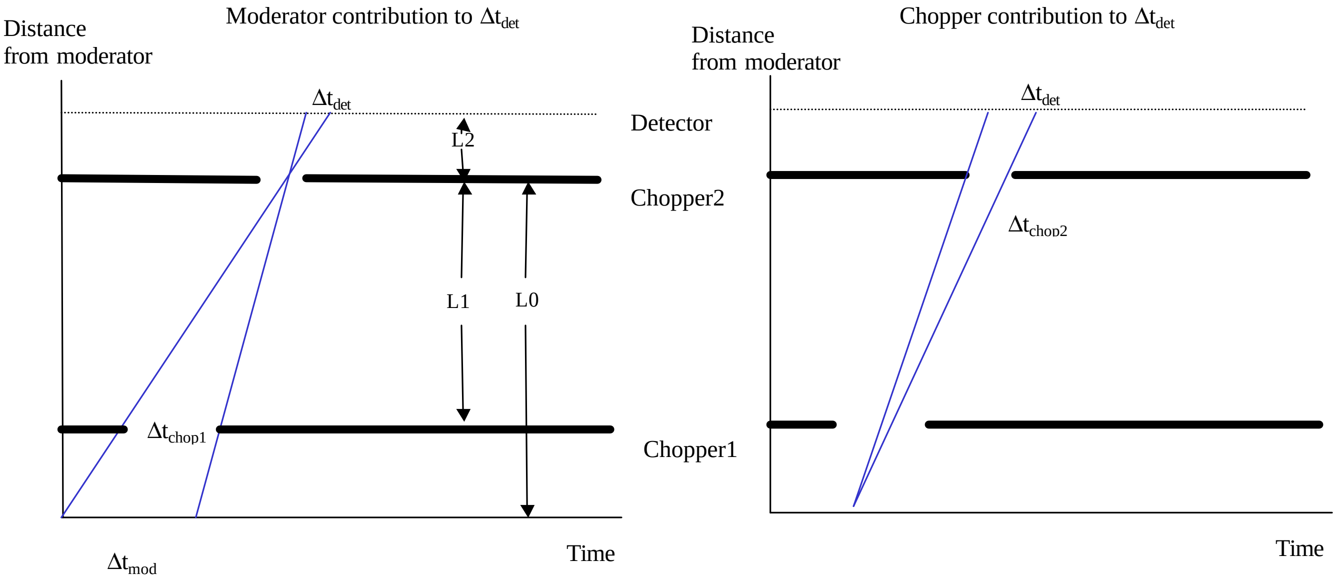
This section describes the main contributions to the energy resolution $R=\varepsilon/E_i$ of the spectrometer, where E_i is the incident energy and ε is the uncertainty in the energy measured.

The energy resolution can be easily calculated and has been written in many forms but I find the most intuitive representation is to write it as

$$R = \frac{\sqrt{E_i}\,\Delta t_{\mathrm{det}}}{1142 L_{sd}}$$

where Δt_{det} is the time uncertainty at the detectors in µs and L_{sd} is the sample to detector distance. There are other contributions to R such as uncertainties in path length due to detector depths and sample size but these tend to be very small compared to the contributions from the moderator and chopper. The equation above gives the energy resolution at the elastic line. The resolution improves with energy transfer ΔE by multiplying the above equation by $(1-\Delta E/E_I)^{3/2}$. In the following all the resolutions quoted will be at the elastic line.

The schematic diagrams below show the contribution of the moderator and chopper components to Δt_{det}



From the above figure it is easy to see from geometric considerations that the time width at the detector due to the moderator is

$$\Delta t_{\mathrm{det}}^{\mathrm{mod}} = \frac{L2}{L1}\Delta t_{chop1}$$

where Δt_{chop1} is the opening time of the1st chopper. L2=L_{sd}+L_{cs} where L_{cs} is the distance from chopper2 to the sample. Δt_{chop1} can be controlled of course so we have control over the moderator width the detector see's. If Δt_{chop1} is larger than the natural width of the moderator then the detector will only see the natural width of course. For the chopper contribution
we have

$$\Delta t_{\mathrm{det}}^{chop} = \frac{L2 + L0}{L0}\Delta t_{chop2}$$

The two time contributions need to be convolved together to give the total time width at the detector Δt_{total}. A good approximation to this to add the two components in quadrature such that

$$\Delta t_{tot} = \left(\Delta t_{\mathrm{det}}^{\mathrm{mod}}\right)^2 + \left(\Delta t_{\mathrm{det}}^{chop}\right)^2$$

From his equation it is clear that one component only has to get slightly bigger and it will dominate the resolution.

3 Chopper optimization (PWR)

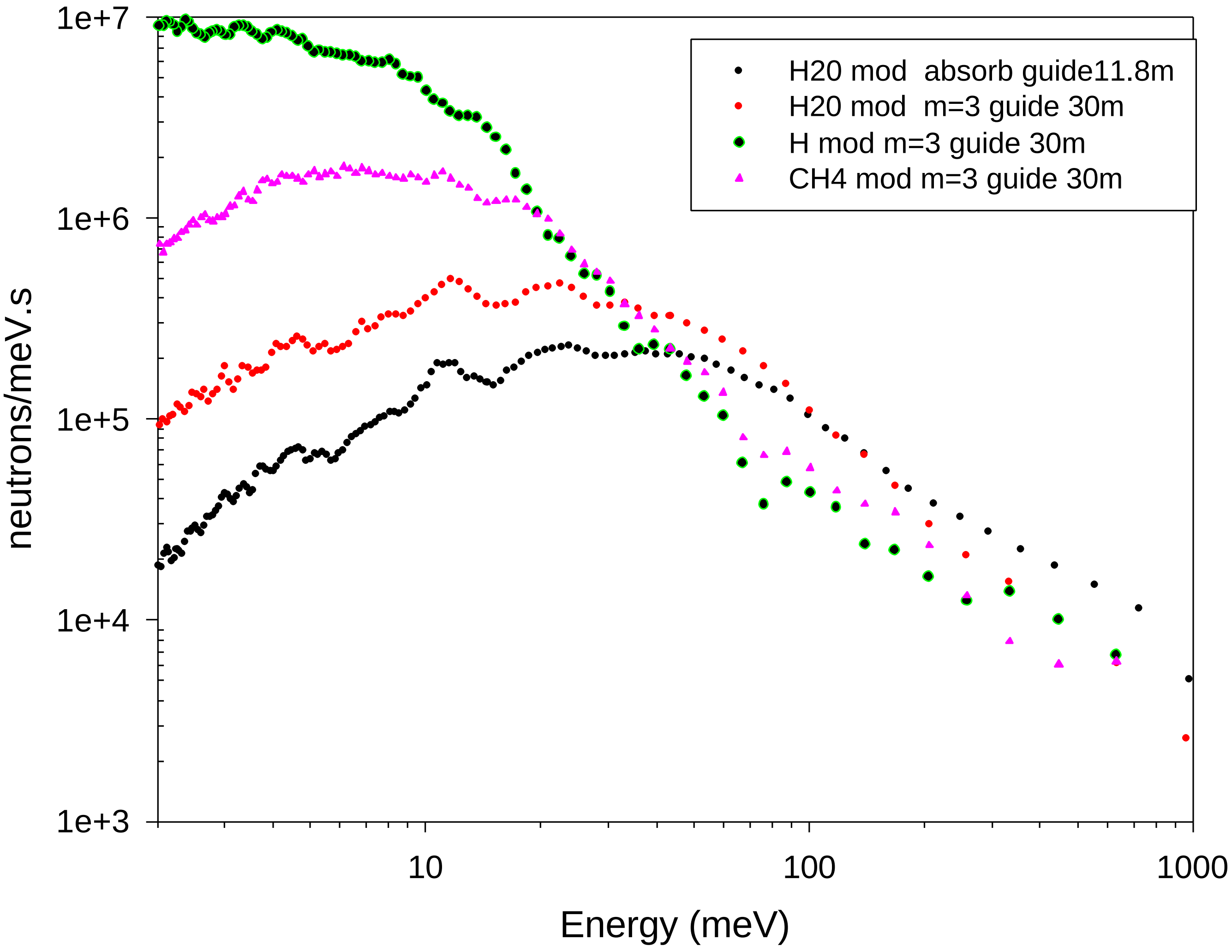
To optimise the total flux for a particular resolution ideally one needs to match the two resolution components at the detector , i.e Δt_{det}^{mod}= Δt_{det}^{chop} .On doing this one gets a condition for the opening times for both choppers to give the maximum possible flux

$$\frac{\Delta t_{chop1}}{\Delta t_{chop2}} = \frac{L2 + L0}{L0}\frac{L1}{L2}$$

R. Lechner who designed NEAT at HMI calls this Pulse-Width Ratio (PWR) optimization. The expression above is slightly different from his expression, as at a reactor the opening time of the 1st chopper directly defines the effective moderator width whereas on a spallation source you need to account for the distance from the moderator to the 1st chopper. If you make L1=L0 you obtain the same result.

4 Choice of moderator

The diagram below shows the flux vs energy for the three moderator types at ISIS

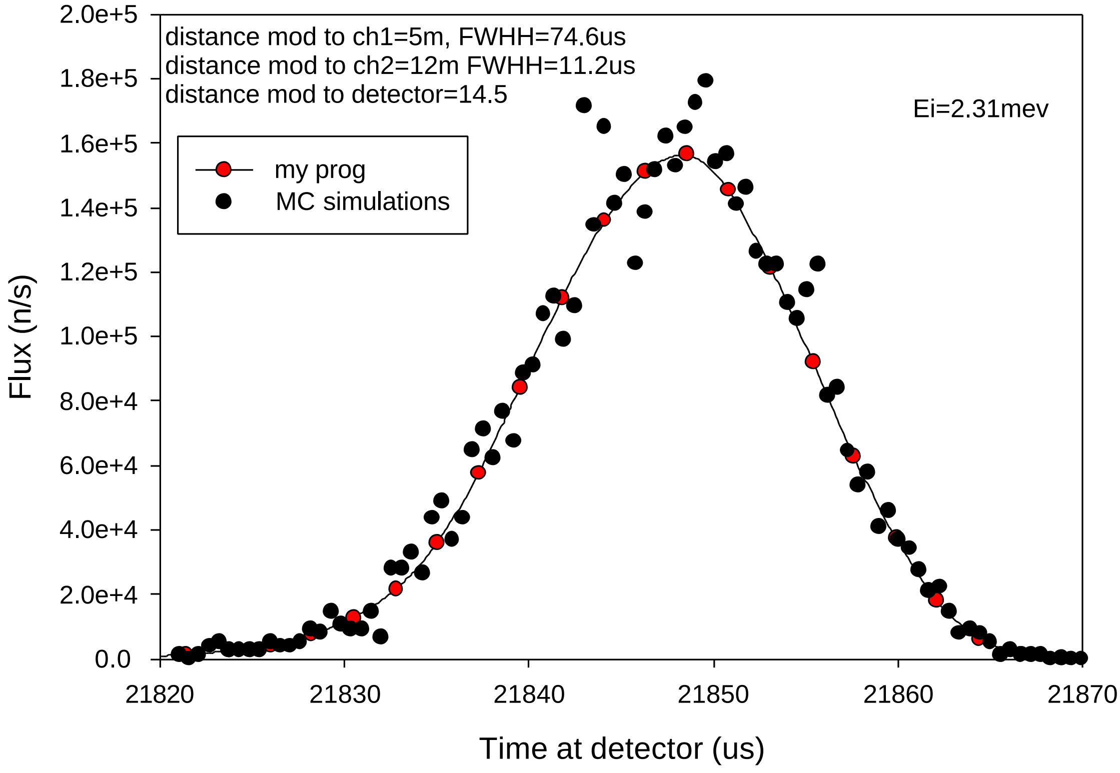


As the design of LET is for energies below 30meV then a hydrogen moderator is the clear choice for maximum flux. The moderators in the above figure are all de-coupled. As we have full control over the moderator time width using the initial chopper then the important parameter is the peak height of the flux. A coupled moderator can typically give you almost double the peak flux of a de-coupled. Also the extra width of the pulse gives you the flexibility to shape the pulse to a nicer triangular resolution lineshape or to relax the resolution and gain a lot more flux. So if one had a choice of moderator then a coupled H would be best.

5 Optimum primary flight path

Higher energy instruments like HET and MAPS tend to be in as close to the moderator as is realistically possible considering all the biological shielding etc. A typical primary flight path of around 10m. This is because of the large$1/r^2$ drop off in flux on these instruments. As LET is a low energy spectrometer the use of a guide changes this argument considerably. In the following discussion and calculation we will show that the optimum L0 is around 20m.

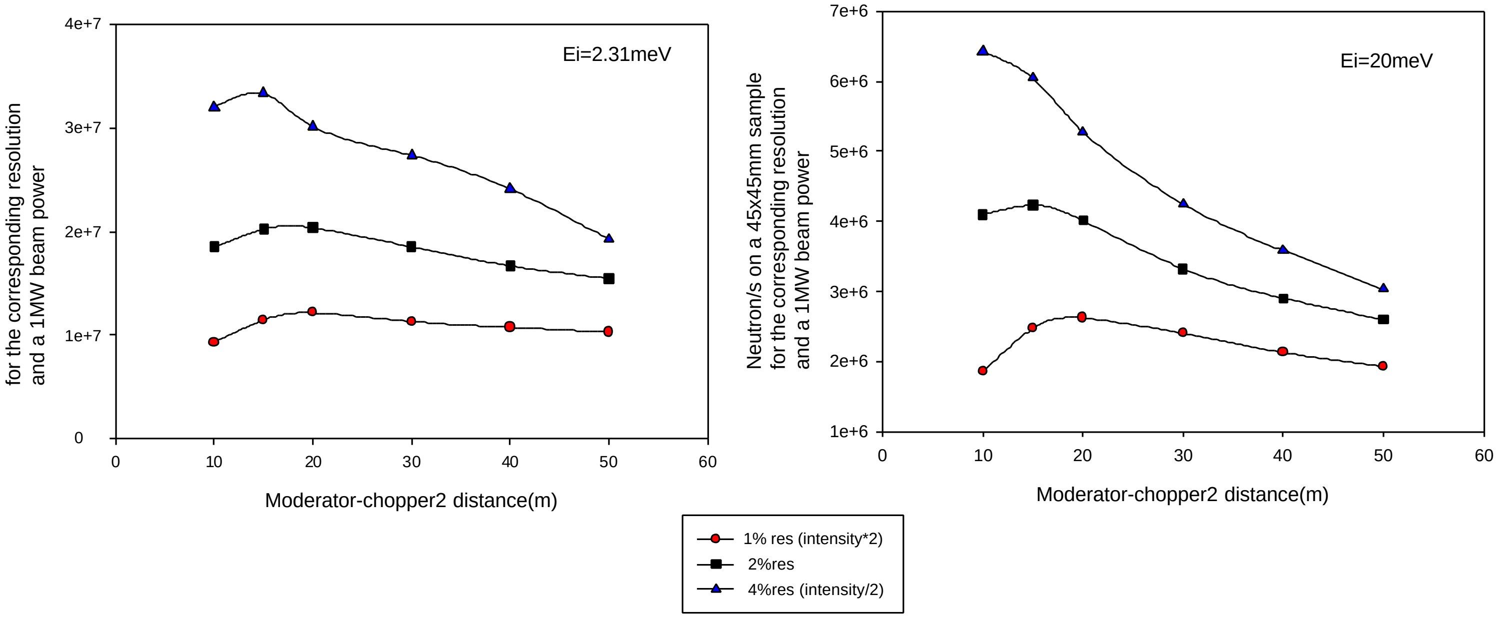
Before continuing to display the results of simulations it is informative to discuss the various parameters affecting the flux on LET. If L0 is very small then to get a particular resolution one finds that Δt_{chop1} has to be very small, i.e we are only chopping a small amount of the available time width of the moderator pulse. Δt_{chop1} gets larger in direct proportion with L0 for the same instrument resolution. Therefore we are cutting more flux from the moderator with increasing L0. As the losses down a guide are very small then it is clear to see that there is an optimum length where for a certain resolution we are utilising the whole moderator width. On increasing L0 further the flux decreases, not only because of the flux losses of the guide but also because the flux accepted from the moderator by chopper2 decreases as 1/L0. This can be seen in the figure 2b. If Δt_{chop2} is kept constant such that the chopper contribution to the resolution is approximately constant, then one can see the acceptance angle of velocities getting through chopper2 is directly proportional to 1/L0. To determine the optimum value for L0, such that we get the best flux for a fixed resolution, I have written a program which calculates the exact amount of flux reaching the detector from every energy and time element on the moderator. This program allows you to vary L0 and chopper opening times etc and see the flux and line shape within seconds. I have tested it against Monte-Carlo simulations using the McLib code and the agreement is excellent, see figure below. The program can be seen in Appendix A.



The figure below shows the flux at the sample position for various values of L0. The resolution was kept fixed for each L0 by varying the values of Δt_{chop1} and Δt_{chop2} as calculated in section 3. The ratio of the chopper opening times was set to maximise the flux at each L0 using the matching condition given in equation *. The relative opening times of the two choppers was also set to focus in time on the peak of the moderator flux. In this case the moderator parameters were for a coupled H moderator who's parameters were supplied by Feri Mezei, see Appendix B for moderator function used in these calculations. Although the resolution calculated from the program at shorter values of L0 was in excellent agreement with the value expected, at longer values of L0 where the full moderator width had already been utilised the program gave a better resolution than calculated. This is to be expected of course as the moderator component contributes less and less to the resolution now. In order to keep a fixed resolution I relaxed the matching condition and opened up the chopper 2 opening time by an amount necessary to still keep the resolution fixed. In the data shown the values of Lcs and Lsd were fixed at 1m and 2.5m respectively. We can see from the figure that the optimum flux for a LET spectrometer would be obtained with a primary path length of about 20m. It is interesting to note that the optimum path length is similar for both values of E_I at 2.27 and 20meV. This is rather fortunate as one length of spectrometer is optimised for the whole energy range of LET. The origin of this is because as E_I increases, then the time width on the detector must decrease to keep the same resolution. This decreases comes about naturally from the fact moderator width also decreases with E_I and therefore L0 does not need to lengthen.

The absolute values of Flux given in the figures were obtained from normalising everything to a Monte-Carlo simulation. The simulation was done for L0= 20m, an m=3 converging guide starting 1m from coupled H moderator (10cm x10cm cross section at moderator down to 4.5cmx4.5cm at sample).

Flux v primary flight path for a fixed resolution
and incident energy



6 LET at the ESS

6.1 Long pulse vs short pulse

As we have already seen an instrument like LET can make use of the full time width of a coupled short pulse moderator by simply increasing the primary flight path, L0. At first sight it may seem that this can be extended such that we increase L0 to such an extent that we utilise the full moderator width of a long pulse.

Two options available for ESS are;

1) 1MW 10Hz short pulse for which we have already analysed in the previous sections
2) 5MW 16.6Hz long pulse (2ms)

The total integrated number of neutrons available at any energy per pulse is 3x that of the 10Hz short pulse option. Or time averaged the increase is a factor of 5. The question is whether are we able to design LET to utilise these extra neutrons.

If we use exactly the same arguments as for the short pulse, with Lsd=2.5m and for a 2% resolution, we find the values of L0 necessary to use the full time width of the long pulse spectrometer are L0=260 and 800m for E_I=2.27 and 20.45meV respectively. The results are summarised below

Short pulse coupled H mod		
E_I (meV)	FWHH of moderator (us)	L0(m) to utilise FWHH
2.27	230	30
20.45	64	25
Long Pulse coupled H mod		
2.27	2000	260
20.45	2000	800

The length of the spectrometer required to use the full 2ms width of the long pulse are ridiculously long and increases rapidly for increasing energies. If we were to force a more reasonable length on the spectrometer say 100m then how do the fluxes compare with the short pulse. Again the information is for a 2% resolution with Lsd=2.5m. The Table below summarises the results

E_I(meV)	Ratio of total Flux long pulse (L0=100m) to Flux short pulse(L0=30m)	Losses over short pulse due to partial use of long pulse width	Losses over short pulse due to the 1/L0 factor	Total losses x Total gain of 5
2.27	0.72	.38	.33	.63
20.45	0.28	.12	.33	.20

These results show that the long pulse option is a not really viable. The results do not even take into account the flux losses down the extra length of guide between the two spectrometers.

7 Fluxes on LET compared to other instruments

In order to make a direct comparison of the capabilities of LET it is important to see what the flux at the sample position would be on LET compared to other similar instruments. For the LET instrument I used the Mclib code. The parameters for the instrument were as follows;

A 10x10cm Coupled H moderator
An m=3 guide starting 1m from moderator and ending 20m from moderator. It converged from 97x97mm down to 45x45mm at sample position. In the code I gave I let the reflectivity be 80% at a critical angle of $3*m_{Ni}$.
Chopper1 was at 5m from moderator
Chopper 2 at 20m from moderator
The chopper opening times were optimised to give the maximum flux at the sample for a certain resolution.

The results and comparison with other instruments are shown below

Ei	NEAT $n/cm^2.s$	IN6 $n/cm^2.s$	LET(ESS1MW) $n/cm^2.s$	LET(ISIS.16MW) $n/cm^2.s$
2.27	$2.0x10^4$ (11%res)	-------	$9.8x10^5$(2%res)	$1.6x10^4$(2%res)
4.86	-------	$8.9x10^4$(3.5%res)	$1.2x10^6$(2%res)	$2.0x10^5$(2%res)
20.45	-------	-------	$1.9x10^5$(2%res)	$3.1x10^4$(2%res)